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Classical description of charge exchange involving He-like or Li-like ions in Rydberg states in plasmas

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Abstract

A purely classical description of energy terms of one-electron Rydberg quasimolecules (hereafter, RQ1) consisting of one electron and two fully stripped ions of charges Z and Z' , where $Z' \neq Z$, had been previously published by one of us. The analysis of the crossings of the energy terms led to a classical description of charge exchange either between a hydrogen-like ion of the nuclear charge Z with a fully stripped ion of the charge Z' or between a hydrogen-like ion of the nuclear charge Z' with a fully stripped ion of the charge Z . Later applications included, e.g., the influence of electric and magnetic fields, as well as of the screening by plasma electrons. In the present paper we extend the classical description of energy terms to *two-electron* Rydberg quasimolecules (RQ2), consisting of two electrons and two fully stripped ions of charges Z and Z' , and to *three-electron* Rydberg quasimolecules (RQ3), consisting of three electrons and two fully stripped ions of charges Z and Z' . We show that classical energy terms of RQ2 and RQ3 also exhibit crossings like the energy terms of RQ1. The crossing of terms of RQ2 occurs at a larger internuclear distance compared to the crossing of the corresponding terms of RQ1, so that the cross-section of the charge exchange for RQ2 is larger than the corresponding cross-section for RQ1. The crossing of terms of RQ3 occurs at an even larger internuclear distance compared to the crossing of the corresponding terms of RQ2, so that the cross-section of the charge exchange for RQ3 is even larger than the corresponding cross-section for RQ2. Thus, the classical roots of charge exchange are revealed not only by the example of RQ1 systems, but also by the examples of RQ2 and RQ3 systems. Our results contribute to advance the understanding of the quantum-classical correspondence and can be used in applications where charge exchange plays the key role.

Keywords: charge exchange, classical description, He-like and Li-like ions, Rydberg quasimolecules

(Some figures may appear in colour only in the online journal)

1. Introduction

Charge exchange has been studied for many decades and continues to be studied because of its great practical importance—see, e.g., books [1, 2]. It affects the feasibility of controlled fusion in magnetic confinement plasma devices, such as, e.g., tokamaks. It is also a controlling factor in ion storage devices. Besides, charge exchange is a mechanism for population inversion in the soft x-ray and

VUV lasers. It plays also an important role in astrophysics.

One of the two mechanisms of charge exchange in plasmas is related to crossings/anticrossings of energy terms of a quasimolecule consisting of the two colliding atoms/ions. A spectroscopic signature of charge exchange in the profiles of spectral lines of multicharged ions is local depressions of the spectral intensity (called x-dips), which offer a method for the experimental determination of the rates

of charge exchange between multicharged ions—see, e.g., review [3] and references therein.

A number of processes in microscopic systems in external fields can be studied classically. These studies contribute to advance the understanding of the quantum-classical correspondence—see, e.g. papers [4–7].

Charge exchange also can be studied within a completely classical description—in addition to quantal studies. In year 2000 one of us published papers [8, 9] presenting a purely classical description of energy terms of Rydberg quasimolecules consisting of one electron and two fully stripped ions of charges Z and Z' , where $Z' \neq Z$. The analysis of the crossings of the energy terms led to a classical description of charge exchange either between a hydrogen-like ion of the nuclear charge Z with a fully stripped ion of the charge Z' or between a hydrogen-like ion of the nuclear charge Z' with a fully stripped ion of the charge Z [8, 9]. This meant that papers [8, 9] broke the paradigm, in which charge exchange was considered an inherently quantum phenomenon.

Later applications of these results included the following studies: the magnetic stabilization of such one-electron Rydberg quasimolecules (hereafter, RQ1) [10], the electric-field-caused enhancement of the ionization of the RQ1 and of charge exchange [11, 12], the effect of the screening by plasma electrons on the classical energy terms of RQ1 [13, 14], the application to the problem of continuum lowering in plasmas [13–15], the effect of a laser field on RQ1 [16], and the attachment of an electron to a muonic hydrogen atom [17, 18] or to a muonic hydrogenic ion [19]. All these studies were summarized in review [20].

In papers [8, 10–14, 17, 18] the studies were focused at Circular Rydberg States (CRS) of the QR1 systems (the analysis in papers [9, 16, 19] went beyond CRS). CRS of atomic and molecular systems, with only one electron, correspond to $l|m| = (n - 1) \gg 1$, where n and m are the principal and magnetic electronic quantum numbers, respectively. They have been extensively studied [21–24] both theoretically and experimentally for several reasons: (a) CRS have long radiative lifetimes and highly anisotropic collision cross sections, thereby enabling experiments on inhibited spontaneous emission and cold Rydberg gases [25, 26], (b) classical CRS correspond to quantal coherent states, objects of fundamental importance, and (c) a classical description of CRS is the primary term in the quantal method based on the $1/n$ -expansion (see, e.g. [27] and references therein).

In the present paper we extend the classical description of energy terms to *two-electron* Rydberg quasimolecules (RQ2), consisting of two electrons and two fully stripped ions of charges Z and Z' , and to *three-electron* Rydberg quasimolecules (RQ3), consisting of three electrons and two fully stripped ions of charges Z and Z' . We show that classical energy terms of RQ2 and RQ3 also exhibit crossings like the energy terms of RQ1. The crossing of terms of RQ2 occurs at a larger internuclear distance compared to the crossing of the corresponding terms of RQ1, so that the cross-section of the charge exchange for RQ2 is larger than

the corresponding cross-section for RQ1. The crossing of terms of RQ3 occurs at an even larger internuclear distance compared to the crossing of the corresponding terms of RQ2, so that the cross-section of the charge exchange for RQ3 is even larger than the corresponding cross-section for RQ2.

2. Analytical calculations of classical energy terms

We consider the following Rydberg quasimolecule: a He-like or Li-like ion of the nuclear charge Z , (having one or two inner electrons in state $1s$, respectively), a highly excited electron in a circular state, and a fully stripped ion of the nuclear charge Z' . (We use atomic units $\hbar = e = m_e = 1$.) The outer electron is in the superposition of the Coulomb potential from charge Z' and the potential Φ_n of a quasinucleus consisting of the nucleus Z and a spherically symmetric charge distribution corresponding to the n inner electrons in the $1s$ state (see, e.g., [28]). For the case $n = 1$, the potential is

$$\Phi_1(r) = \frac{Z - 1}{r} + \left(Z\mu + \frac{1}{r} \right) e^{-2Z\mu r} \quad (1)$$

and for the case $n = 2$, the potential is (see, e.g., book [29])

$$\Phi_2(r) = \frac{Z - 2}{r} + 2 \left(\left(Z - \frac{5}{16} \right) \mu + \frac{1}{r} \right) e^{-2 \left(Z - \frac{5}{16} \right) \mu r}, \quad (2)$$

where $\mu = Mm/(M + m)$ is the reduced mass of the pair ‘nucleus Z —electron’, M is the nuclear mass, and r is the radial coordinate. In both cases the additional term in the total potential (compared to the Coulomb potential) corresponds to the potential due to the spherically symmetric charge distribution of the n inner electrons in the $1s$ state.

The classical Hamilton function (for brevity, Hamiltonian) of the highly excited electron is

$$H = \frac{1}{2} \left(p_z^2 + p_\rho^2 + \frac{p_\phi^2}{\rho^2} \right) - \Phi_n(r) - \frac{Z'}{\sqrt{\rho^2 + (R - z)^2}}, \quad (3)$$

where $r = (\rho^2 + z^2)^{1/2}$ is the distance from the highly excited electron to the nucleus Z and (ρ, φ, z) are the cylindrical coordinates such chosen that the nuclei Z and Z' are on the z -axis at $z = 0$ and $z = R$, respectively. Since the electron is in a circular state, then φ is a cyclic coordinate and its corresponding momentum is conserved:

$$p_\phi = \rho^2 \frac{d\phi}{dt} = L. \quad (4)$$

With (4) and (1) or (2) substituted into (3), we obtain

$$H = \frac{1}{2} \left(p_z^2 + p_\rho^2 \right) + E, \quad (5)$$

where, for the case $n = 1$, we get

$$E = \frac{L^2}{2\rho^2} - \frac{Z-1}{\sqrt{\rho^2+z^2}} - \left(Z\mu + \frac{1}{\sqrt{\rho^2+z^2}} \right) e^{-2Z\mu\sqrt{\rho^2+z^2}} - \frac{Z'}{\sqrt{\rho^2+(R-z)^2}} \quad (6)$$

and for $n = 2$ we get

$$E = \frac{L^2}{2\rho^2} - \frac{Z-2}{\sqrt{\rho^2+z^2}} - 2\left(\left(Z - \frac{5}{16} \right) \mu + \frac{1}{\sqrt{\rho^2+z^2}} \right) e^{-2\left(Z - \frac{5}{16} \right) \mu \sqrt{\rho^2+z^2}} - \frac{Z'}{\sqrt{\rho^2+(R-z)^2}}. \quad (7)$$

In a circular state, $p_z = p_\rho = 0$, and E becomes the total energy of the electron.

Using the scaled quantities

$$\ell = \frac{L}{\sqrt{ZR}}, \quad w = \frac{z}{R}, \quad v = \frac{\rho}{R}, \quad p = v^2, \quad \varepsilon = -\frac{R}{Z}E, \quad k = \mu R, \quad b = \frac{Z'}{Z}, \quad r = \frac{Z}{L^2}R \quad (8)$$

and combining the two cases, we obtain the scaled energy ε of the electron for both cases $n = 1$ and $n = 2$:

$$\varepsilon = \frac{1 - \frac{n}{Z}}{\sqrt{w^2+p}} + \frac{b}{\sqrt{(1-w)^2+p}} + \frac{n}{Z} \times \left(\left(Z - \frac{5(n-1)}{16} \right) k + \frac{1}{\sqrt{w^2+p}} \right) \times e^{-2\left(Z - \frac{5(n-1)}{16} \right) k \sqrt{w^2+p}} - \frac{\ell^2}{2p}. \quad (9)$$

Note that this formula corresponds to the case of RQ1 [1, 2] when $n = 0$. From the equilibrium on the scaled coordinates (w, p) we require

$$\frac{\partial \varepsilon}{\partial w} = 0, \quad \frac{\partial \varepsilon}{\partial p} = 0. \quad (10)$$

The first of the two derivatives in equation (10) being equated to zero, yields the equilibrium relation between the coordinates (w, p) for the given values of Z, b and k . The

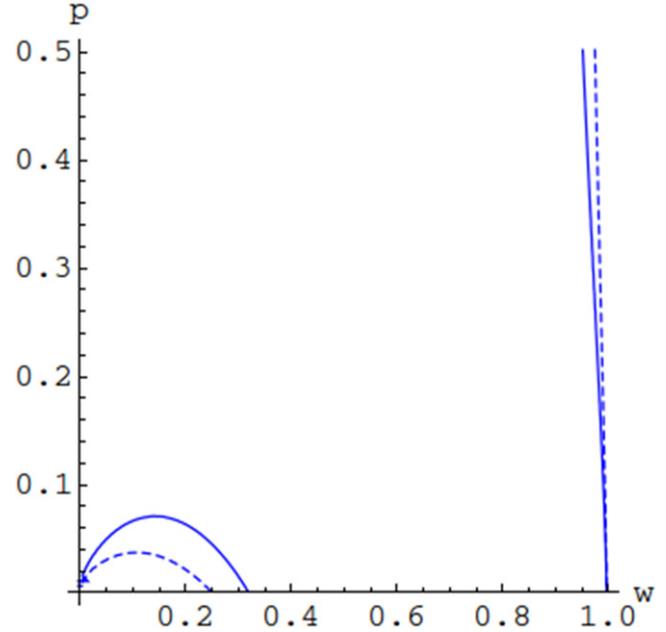


Figure 1. Equilibrium plot of the dependence of the squared scaled radius of the orbit p on the scaled axial coordinate w for $Z = 3$, $b = 3$, $k = 10$, for $n = 1$ (solid curves) and $n = 2$ (dashed curves).

explicit form of this relation is as follows:

$$\frac{b(1-w)}{w((1-w)^2+p)^{3/2}} = \frac{1 - \frac{n}{Z}}{(w^2+p)^{3/2}} + \frac{n}{Z} \frac{1 + 2\left(Z - \frac{5(n-1)}{16} \right) k \sqrt{w^2+p} \left(1 + \left(Z - \frac{5(n-1)}{16} \right) k \sqrt{w^2+p} \right)}{(w^2+p)^{3/2}} \times e^{-2\left(Z - \frac{5}{16} \right) k \sqrt{w^2+p}}. \quad (11)$$

Figure 1 shows, as an example, the plot $p(w)$ for $Z = 3$, $b = 3$, $k = 10$, for both cases $n = 1$ and $n = 2$.

As in the case of RQ1 [1, 2], the equilibrium range is $0 < w < w_1$ and $w_3 < w < 1$. In the present case,

$$w_1 = \frac{\alpha}{\left(Z - \frac{5(n-1)}{16} \right) k}, \quad (12)$$

where α is the solution of the transcendental equation

$$\frac{b\alpha^2}{\left(\left(Z - \frac{5(n-1)}{16} \right) k - \alpha \right)^2} = 1 + \frac{n}{Z} \left(\left(1 + 2\alpha + 2\alpha^2 \right) e^{-2\alpha} - 1 \right). \quad (13)$$

The value of w_1 is typically about 0.3, Z is between 1 and Z_{\max} , where $Z_{\max} \sim 10$. The value of μ is very close to 1 (details are in equation (19)), so that $k = \mu R \approx R = (L^2/Z)r$. Therefore, $\alpha \approx wZk \approx wZ(L^2/Z)r = wL^2r \approx (L^2/3)r$, which for the excited electron and most values of the scaled

internuclear distance is a number significantly greater than 1. Thus, the term in equation (13) with the exponential function can be neglected, and this approximation yields (using equation (12))

$$w_1 \approx \frac{1}{1 + \sqrt{\frac{b}{1 - \frac{n}{Z}}}}. \quad (14)$$

In the case of two bare nuclei ($n = 0$), equation (14) yields the result obtained in [1, 2]: $1/(1 + b^{1/2})$.

The asymptote $w = w_3$ is determined by

$$w_3 = \frac{b}{b + 1 - \frac{n}{Z}}. \quad (15)$$

While calculating the second out of the two derivatives in equation (10), the last term in equation (9) survives. It contains the equilibrium value of ℓ . We subtract the first derivative (equation (11)) from the second one and obtain the value of the scaled angular momentum in the circular state:

$$\ell^2 = \frac{bp^2}{w((1-w)^2 + p)^{3/2}}. \quad (16)$$

From the scaling formulas (8) it follows that $r = 1/\ell^2$, that is,

$$r = \frac{w((1-w)^2 + p)^{3/2}}{bp^2}. \quad (17)$$

Substituting equation (16) into equation (9), we obtain the scaled energy:

$$\begin{aligned} \varepsilon = & \frac{1 - \frac{n}{Z}}{\sqrt{w^2 + p}} + b \frac{(1-w)^2 + p \left(1 - \frac{1}{2w}\right)}{\left((1-w)^2 + p\right)^{3/2}} \\ & + \frac{n}{Z} \left(\left(Z - \frac{5(n-1)}{16} \right) k + \frac{1}{\sqrt{w^2 + p}} \right) \\ & \times e^{-2 \left(Z - \frac{5(n-1)}{16} \right) k \sqrt{w^2 + p}}. \end{aligned} \quad (18)$$

From equation (8), $k = \mu R$, where μ is the reduced mass of the pair nucleus—electron. In our units, the mass of the electron is 1, so $\mu = M/(1 + M)$, where M is the nuclear mass $Zm_p + Nm_n$ of the nucleus containing Z protons and N neutrons. In atomic units, $m_p \approx 1849.3596$ and

$m_n \approx 1851.9088$. Since

$$\begin{aligned} \mu &= \frac{M}{1 + M} = \frac{1}{\frac{1}{M} + 1} = \frac{1}{\frac{1}{Zm_p + Nm_n} + 1} \\ &\approx \frac{1}{\frac{1}{(Z + N)m_p} + 1}, \end{aligned} \quad (19)$$

the lower limit of μ is realized when $Z = 1$ and $N = 0$ and is approximately 0.999 46 and the upper limit is 1. Therefore, the realistic values of μ lie in the range $0.999 46 \leq \mu < 1$. The values of R for the case of a Rydberg quasimolecule are of the order of several Bohr radii. Thus, the realistic values of $k = \mu R$, which is physically the slightly scaled internuclear distance, are somewhere between 1 and 10.

The last term in equation (11) containing the exponential function is small and can be neglected, leading to the possibility of an analytical solution. This equation can then be solved for p , which can then be substituted into equations (18) and (17), thus obtaining the equilibrium equations for ε and r . Also, from the scaling formulas we see that $E = -(Z/L)^2 \varepsilon/r$, so that if we denote $\varepsilon/r = \varepsilon_1$, then ε_1 and r will have the same scaling. Thus, we obtain the parametric dependence $\varepsilon_1(r)$ for the given b, r, Z, L, N, n with the parameter w taking all values in the allowed range $0 < w < w_1, w_3 < w < 1$ according to equations (14) and (15). This dependence can be simplified further by introducing the parameter [13]

$$\gamma = \left(\frac{1}{w} - 1 \right)^{1/3}. \quad (20)$$

The final parametric approximate analytical dependence can be represented by the following formulas (21) and (22):

$$\begin{aligned} \varepsilon_1 = & \left(1 - \frac{n}{Z} \right) \frac{\gamma(c^{2/3} - \gamma^4)^2}{\gamma^6 - 1} \\ & \times \left(\left(1 - \frac{n}{Z} \right) \frac{\gamma(\gamma^3 - 2) + c^{2/3}(2\gamma^3 - 1)}{2\gamma(\gamma^3 - 1)^2} + \frac{n}{Z} \right) \\ & \times \left(\frac{1}{\gamma^3 - 1} + \mu L^2 \frac{1 - \frac{5(n-1)}{16Z}}{1 - \frac{n}{Z}} \frac{\gamma^6 - 1}{(c^{2/3} - \gamma^4)^2} \right) \\ & \times e^{-2\mu L^2 \frac{1 - \frac{5(n-1)}{16Z}}{1 - \frac{n}{Z}} \frac{(\gamma^6 - 1)^2}{\gamma(\gamma^3 + 1)(c^{2/3} - \gamma^4)^2}}. \end{aligned} \quad (21)$$

$$r = \frac{1}{1 - \frac{n}{Z}} \frac{(\gamma^6 - 1) \sqrt{c^{2/3} \gamma^2 - 1}}{\gamma(c^{2/3} - \gamma^4)^2}, \quad (22)$$

where

$$c = \frac{b}{1 - \frac{n}{Z}} \quad (23)$$

and the parameter γ takes all values in the allowed range $0 < \gamma < 1/c^{1/3}$, $c^{1/6} < \gamma < +\infty$.

In figures 2 and 3 we present the classical energy terms $\varepsilon_1(r)$ for the case $b = 3, Z = 6, N = 6, L = 10$ in the cases of RQ2 or RQ3 in comparison with the case of RQ1 [1, 2] shown in red, thinner curves.

We also performed an exact numerical solution to this problem. From the scaling formula for $R, k = (\mu L^2/Z)r$ with μ given by equation (19). Equation (17), after being squared, is a fourth-degree polynomial with respect to p and has a real positive analytical solution for p which depends on r : $p_0 = p(w, b, r)$. Substituting k and the solution for p into equations (18) and (11), we obtain the formula for energy $\varepsilon(w, b, r, Z, L, N, n)$ and equation (11) bearing the same variables. Then we solve the resulting equation (11) for w (it may have up to 3 solutions) and substitute them into $\varepsilon(w, b, r, Z, L, N, n)$. Also, from the scaling formulas we see that $E = -(Z/L)^2 \varepsilon/r$, so if we denote $\varepsilon/r = \varepsilon_1$, then ε_1 and r will have the same scaling. Thus, we obtain the energy $\varepsilon_1(b, r, Z, L, N, n)$, which yields the classical energy terms $\varepsilon_1(r)$ for the given values of b, Z, L and N , for $n = 1, 2$.

We made the numerical plots for the cases $b = 3, Z = 6, N = 6, L = 10, n = 1, 2$ and compared them to the analytical plots for the same cases. As seen from figures 4 and 5, the exact (numerical) classical energy terms coincide with the approximate analytical ones.

The analysis of the difference between the approximate and exact values for p and r shows a vanishingly small error (less than 10^{-10}) in almost all cases considered. Also, we measured the time it takes to build a numerical plot and compared it to that of building an analytical plot. The ratio of the first to the second was found to be about 2500, which shows the efficiency of the analytical solution.

3. Relation to charge exchange

When $Z_{\text{eff}} = Z - n$ and Z' differ significantly from each other, the V-type crossings occur between two classical energy terms that can be asymptotically labeled as Z_{eff} - and Z' -terms. This situation *classically depicts charge exchange*, as explained in papers [1, 2]. Indeed, say, initially at $r \rightarrow \infty$, the electron was a part of the ion of the nuclear charge $Z_{\text{min}} = \min(Z', Z_{\text{eff}})$. As the charges Z_{eff} and Z' come relatively close to each other, the two terms undergo a V-type crossing and the electron is shared between the Z_{eff} - and Z' -centers. Finally, as the charges Z_{eff} and Z' go away from each other, the electron ends up as a part of the ion of the nuclear charge $Z_{\text{max}} = \max(Z', Z_{\text{eff}})$.

For collisions with relatively low velocities, the classical cross-section of charge exchange can be calculated using the

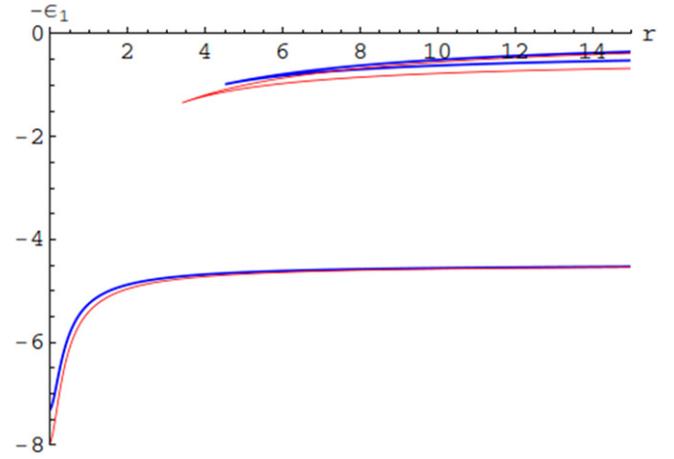


Figure 2. Classical energy terms $\varepsilon_1(r)$ for the case of RQ2 for $b = 3, Z = 6, N = 6, L = 10$ (blue, thick) and the corresponding terms for the case of RQ1 (red, thin), which are lower than their counterparts in RQ2. RQ1 and RQ2 stand for Rydberg quasimolecules with 1 or 2 electrons, respectively.

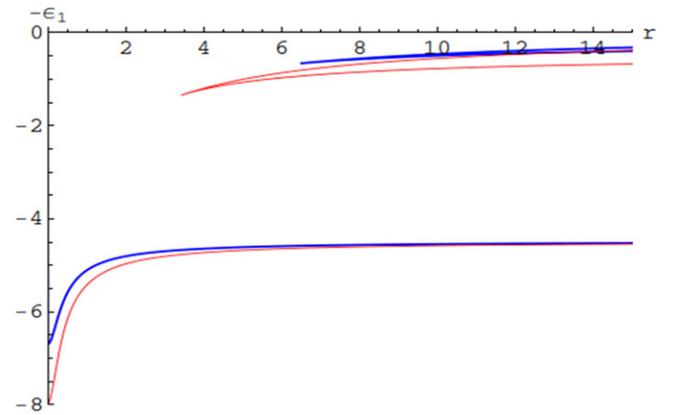


Figure 3. Classical energy terms $\varepsilon_1(r)$ for the case of RQ3 for $b = 3, Z = 6, N = 6, L = 10$ (blue, thick) and the corresponding terms for the case of RQ1 (red, thin), which are lower than their counterparts in RQ3. RQ1 and RQ3 stand for Rydberg quasimolecules with 1 or 3 electrons, respectively.

impact parameter method (see, e.g., book [30]). In the integral over the impact parameters, the overwhelming contribution comes from the vicinity of the crossing of the energy terms. Therefore, the corresponding cross-section is proportional to the square of the crossing distance.

From figure 2 it is seen that the V-type crossing of the upper two terms for RQ2 occurs at a larger internuclear distance than for RQ1. Therefore the cross-section of the charge exchange for RQ2 is larger than the corresponding cross-section for RQ1.

From figure 3 it is seen that the V-type crossing of the upper two terms for RQ3 occurs at an even larger internuclear distance than for RQ2. Therefore the cross-section of the charge exchange for RQ3 is even larger than the corresponding cross-section for RQ2.

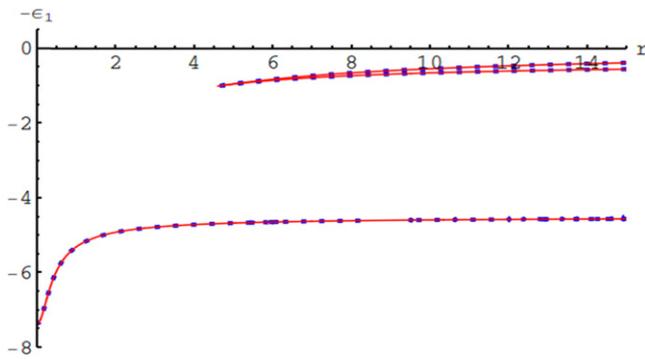


Figure 4. Classical energy terms $\varepsilon_1(r)$ for the case of RQ2 for $b = 3$, $Z = 6$, $N = 6$, $L = 10$ obtained from the analytical (solid, red curves) and numerical (dotted, blue curves) solutions.

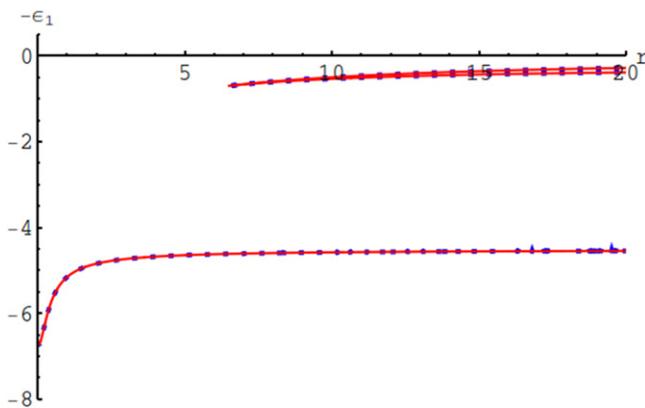


Figure 5. Classical energy terms $\varepsilon_1(r)$ for the case of RQ3 for $b = 3$, $Z = 6$, $N = 6$, $L = 10$ obtained from the analytical (solid, red curves) and numerical (dotted, blue curves) solutions.

4. Conclusions

We extended the classical description of energy terms from one-electron Rydberg quasimolecules (RQ1) to two-electron Rydberg quasimolecules (RQ2) and to three-electron Rydberg quasimolecules (RQ3). We obtained the classical energy terms of RQ2 and of RQ3, and found that they exhibit crossings like the energy terms of RQ1.

We explained the relation between the crossings of the classical energy terms and charge exchange. Thus, the classical roots of charge exchange have been revealed not only by the example of RQ1 systems, as in papers [1, 2], but also by the examples of RQ2 and RQ3 systems.

The crossing of terms of RQ2 occurs at a larger internuclear distance compared to the crossing of the corresponding terms of RQ1, so that the cross-section of the charge exchange for RQ2 is larger than the corresponding cross-section for RQ1. The crossing of terms of RQ3 occurs at an

even larger internuclear distance compared to the crossing of the corresponding terms of RQ2, so that the cross-section of the charge exchange for RQ3 is even larger than the corresponding cross-section for RQ2.

From the fundamental point of view, our results contribute to advance the understanding of the quantum-classical correspondence (for example of which we referred to papers [4–7]). From the practical point of view, our results can be used in applications where charge exchange plays the key role, such as, e.g., the phenomenon of x-dips in profiles of spectral lines from plasmas [3].

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